Procedures for performing QA checks within ChemFinder Main Database (ver. 7.0 for Windows) *(25 November 03)*

**Note: Main Database for development purposes has two structure fields corresponding to the tested form and DOP (defined organic parent) form. Structure, SMILES and CAS correspond to tested form; Structure_DOP, SMILES_DOP and CAS_DOP correspond to simplified parent form for defined organics only.*

1. Open Main ChemFinder file.
2. **CTRL+F** opens blank record page for search query.
3. Type search query into appropriate field, using * before text for wildcard.
4. Result of search will retrieve all records satisfying query, with number of found records indicated in lower right bottom of screen.
5. Click on Main Menu **Search → Retrieve All** to return to complete database for new search.
6. Perform the following count checks:
   a. TestedForm: parent, salt, complex (complex, salt complex)
      i. Total + mixture count should equal Database Total
   b. SubstanceType: defined organic, inorganic, organometallic, mixture or unknown
      i. Total should equal Database Total
7. Other visual checks, in main table view:
   a. Search for all SubstanceType:defined organic
      i. Within this subset choose table view
      ii. Should be no blank Structure fields
      iii. Should be no blank SMILES or SMILES_DOP fields
   b. Return to form view, still within defined organic subset
      i. Search for TestedForm "salt or complex", verify count, go to table view
      ii. No AddToParent field should be blank, check entries
      iii. CAS and CAS_DOP should be different in all cases
      iv. SMILES and SMILES_DOP should be different in all cases
      v. Structure and Structure_DOP should be different in all cases
   c. Return to form view, retrieve all, search for SubstanceType:defined organic and TestedForm:parent simultaneously, choose table view
      i. AddToParent fields should all be blank
      ii. CAS and CAS Parent should be identical in all cases
      iii. SMILES and SMILES Parent should be identical in all cases
      iv. Structure and Structure Parent should be identical in all cases
   d. Return to form view, retrieve all, search for SubstanceType:inorganic, choose table view
      i. Structure_DOP, CAS_DOP, SMILES_DOP, AddtoParent fields should all be blank
   e. Return to form view, retrieve all, search for SubstanceType:organometallic, choose table view
      i. Structure_DOP, CAS_DOP, SMILES_DOP, AddtoParent fields should all be blank

ii. TestedForm field should all be "complex"

f. Return to form view, retrieve all, search for SubstanceType:mixture, choose table view

i. Structure, Structure_DOP, CAS_DOP, SMILES, SMILES_DOP, AddToParent fields should all be blank

ii. CAS can have non-blank entry

iii. ChemNote field used to distinguish defined mixture (e.g., mixture of isomers) from unknown substances (i.e., undefined mixture, unknown structure)

8. SMILES generation and checks for main tested form and DOP Structures

a. Within main form view of ChemFinder application, right click on structure field to "Copy as SMILES", go to appropriate SMILES field and paste [CTRL+V]

b. Within main form view of ChemFinder, copy SMILES field entry, go to blank structure field, right click and choose "Paste SMILES"

c. Can Paste SMILES into ChemDraw application to generate structure, as well

9. ChemName, CAS checks for tested form and DOP Structures

a. http://chemfinder.cambridgesoft.com/ used to verify tested form ChemName, CAS, and Structure

b. http://chemfinder.cambridgesoft.com/ used to search for CAS_DOP for simplified form of salts and complexes, verify using Structure_DOP

10. Additional check for valid structures can be performed by following Procedure for import of SDF into ACD ChemFolder, where if the Import Option for Importing Invalid Structures is left unchecked, only valid structures will be imported. The total record count after import should equal the total record count of valid structures in the original database. Note that this count will exclude all "mixture or unknown" records.

11. Checks for valid SMILES to structure conversions can be done by following procedure for import of SDF into Excel, as in the creation of DOP file, deleting structure field, copying and converting SMILES field to structure. **Caution:** be sure to copy files to a separate Test folder for this check.

12. Checks of ChemNote field:

a. Search for all instances of N+ in SMILES or SMILES parent field and check to see that "quaternary ammonium" written in ChemNote field if applicable

b. Search for all instances of stereospecificity in structure, e.g. *cis, trans, E, Z, R, S, endo, exo, syn, anti, confirming with visual check of names; for all cases enter "stereochem" in ChemNote field.